

CL2001 US NA

What is claimed is:

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1. A computer-controlled reaction apparatus for simultaneously conducting chemical reactions on a plurality of samples by maintaining the samples in chemical isolation from each other and subjecting each of the samples to substantially identical conditions, comprising:

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(a) a generally cylindrical reactor housing having a bore and a central axis, the housing comprised of:

i) a loading/unloading section having an airlock;

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ii) a reaction section;

iii) an analytical monitoring system;

iv) a drive section;

v) a distribution manifold system;

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(b) a gas-distribution and pressure control system in communication with the reactor housing;

(c) a positioning system connected to the drive section;

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(d) a temperature control system for controlling the temperature of the reactor housing;

(e) a reaction assembly, contained within the reactor housing, and movable in the housing bore in a direction along

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the axis of the housing, the reaction assembly comprising:

i) a cylindrical outer body having a bore, a plurality of ports and a fluid distribution manifold;

ii) a cylindrical inner body contained within the bore of the outer body and having:

A) a bore and a plurality of ports, and

B) a sample holder containing a plurality of sample holding positions for containing the samples to be reacted,

the sample holder being receivable within the bore of inner body and movable along the axis to a fully-inserted position, wherein, when the sample holder is in the fully-inserted position within the inner body, each of the plurality of reaction wells is aligned with each of the plurality of ports of the inner body;

(f) an analytical monitoring system comprising: at least one optical port and at least one optical arrangement, comprising a paired source and detector, the at least one optical arrangement being capable of performing a measurement, at one or more ultraviolet, visible or infrared wavelengths, of a sample contained at a sample holding position to characterize the sample;

(g) a computer controller, connected to the gas-distribution and pressure control system, the positioning system, the temperature control system, and the analytical monitoring system;

wherein the reaction assembly is movable between the loading/unloading section, the reaction section, and the analytical monitoring system; and

wherein the drive section mechanically links the reaction assembly to the positioning system, so that the reactor assembly is positioned to each of a plurality of predetermined

monitoring positions, such that at least one of the reaction wells is aligned with the at least one analytical port at each of the plurality of monitoring positions.

5        2. The apparatus of claim 1 wherein the computer controller comprises a central processor, connected by a data bus to a random access memory (RAM), a data storage device, an interface subsystem and a display device, the central processor being controlled by an operating system and  
10 application software stored in the data storage device, the central processor controlling the interface subsystem which is connected to, and controls, the gas-distribution and pressure control system, the positioning system, the temperature control system, and the optical monitoring system.

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      3. The apparatus of claim 1 wherein the gas-distribution and pressure control system comprises a supply of one or more gases, one or more valves and associated flow measuring devices and pressure regulators for controlling the flow of  
20 gas to the reaction assembly.

      4. The apparatus of claim 1, wherein the temperature control system comprises one or more heating elements, one or more temperature sensors and a control unit, the control unit  
25 being electrically connected to the interface subsystem of the computer controller for receiving a temperature control signal and being connected to the one of more sensors for receiving temperature signals and being connected to the one of more heating elements for controlling electrical current to said  
30 heating elements.

      5. The apparatus of claim 1 wherein the optical ports of the optical monitoring system are positioned in a coplanar arrangement so that an optical arrangement, comprising one or

more ports, a optical source and an optical detector may be selected from a plurality of optical arrangements for characterizing each sample.

5           6. The apparatus of claim 1 wherein the optical monitoring system comprises a spectrophotometer.

7. The apparatus of claim 1 wherein the optical arrangement comprises a transmission arrangement, wherein  
10 light is transmitted through the thin film samples.

8. The apparatus of claim 1 wherein the optical arrangement comprises a reflection arrangement, wherein light is reflected from at least one surface of the thin film  
15 samples.

9. The apparatus of claim 1 wherein the optical arrangement comprises an attenuated total reflection arrangement, wherein light is repeatedly reflected from a  
20 surface of the thin film samples.

10. A method of performing a plurality of chemical reactions using the apparatus of Claim 1, comprising the steps  
of:

25           (a) positioning the reactor assembly at an initial undocked position in the loading/unloading section, loading the sample holder with samples to be reacted and inserting the sample holder into the inner body of the reactor assembly and closing the airlock,

30           (b) moving the inner body of the reactor assembly to a docked position within the outer body,

          (c) causing the temperature control system to bring the reactor assembly to a predetermined temperature,

(d) causing the fluid distribution and pressure control system to introduce one or more reactant fluids at a predetermined flow rate and pressure to the samples within the sample holding positions,

5 (e) maintaining the fluid flow and pressure for a predetermined time so that a reaction occurs between the reactant fluids and the samples,

(f) sequentially positioning the reactor assembly so that each of the sample positions is aligned at each of the plurality of monitoring positions,

10 (g) performing at least one optical measurement to characterize each sample,

(h) returning the reactor assembly to the initial position in the loading/unloading section,

15 (i) quenching the reaction by stopping the flow of reactant fluids and initiating a flow of quenching gas to return the temperature and pressure of the reaction assembly to ambient,

(j) moving the inner body of the reactor assembly to the undocked position, and

20 (k) opening the airlock and removing the sample holder from the reactor assembly.

11. A method for testing a plurality of samples,  
25 comprising (a) simultaneously reacting all samples with a fluid, and (b) during the reaction of the samples with the fluid, subjecting each sample in sequence to analysis.

12. The method of Claim 11 wherein the reaction of the  
30 samples with the fluid and the analysis are performed in a sealed vessel, and the method further comprises, while the samples remain in the sealed vessel, subjecting one or more of them to a second simultaneous reaction with a fluid, and a second analysis.

13. A method according to Claim 11 wherein the analysis is optical analysis.

5        14. A method according to Claim 11 wherein the analysis is selected from the group consisting of ultrasonic, electrostatic, magnetic, radio frequency or x-ray analysis.

10       15. A method according to Claim 11 wherein each sample is reacted with the fluid in a chamber in which the temperature or the pressure is controlled.

15       16. A method according to Claim 11 wherein each sample is reacted with the fluid in a first chamber, and each sample is subjected to analysis in a second chamber, and the first chamber is isolated from the second chamber.

20       17. A method for testing a plurality of samples, comprising (a) simultaneously reacting all samples with a fluid in a sealed vessel, and (b) after completion of the reaction of the samples with the fluid, subjecting each sample in sequence to analysis in the sealed vessel.

25       18. A method according to Claim 17 wherein the analysis is optical analysis.

30       19. A method according to Claim 17 wherein the analysis is selected from the group consisting of ultrasonic, electrostatic, magnetic, radio frequency or x-ray analysis.

20. A method according to Claim 17 wherein each sample is reacted with the fluid in a chamber in which the temperature or the pressure is controlled.

21. A method according to Claim 17 wherein each sample is reacted with the fluid in a first chamber, and each sample is subjected to analysis in a second chamber, and the first chamber is isolated from the second chamber.

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22. A method for testing a group of samples, comprising (a) simultaneously reacting all samples with a fluid in a sealed vessel, (b) before or after step (a), simultaneously reacting one or more members of a subgroup of the group of samples with a fluid in the sealed vessel, and (c) subjecting each sample to analysis.

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23. A method according to Claim 22 wherein the analysis is optical analysis.

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24. A method according to Claim 22 wherein the analysis is selected from the group consisting of ultrasonic, electrostatic, magnetic, radio frequency or x-ray analysis.

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25. A method according to Claim 22 wherein each of the samples, or each of the members of the subgroup of samples, is reacted with the fluid in a chamber in which the temperature or the pressure is controlled.

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26. A method according to Claim 22 wherein each sample is reacted with the fluid in a first chamber, and each sample is subjected to analysis in a second chamber, and the first chamber is isolated from the second chamber.

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27. A method for testing a plurality of samples, comprising (a) bringing all samples to a predetermined temperature in a first chamber of a vessel, (b) simultaneously exposing each sample in a second chamber of the vessel, which

is isolated from the first chamber, to a reactive fluid, and  
(c) subjecting each sample to analysis.

28. A method according to Claim 27 further comprising a  
5 step, after completion of analysis, of changing in the first  
chamber the temperature of all samples to a temperature above  
or below the predetermined temperature.

29. A method according to Claim 27 wherein the analysis  
10 is optical analysis.

30. A method according to Claim 27 wherein the analysis  
is selected from the group consisting of ultrasonic,  
electrostatic, magnetic, radio frequency or x-ray analysis.  
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31. A method according to Claim 27 wherein each sample  
is subjected to analysis in a third chamber, and the third  
chamber is isolated from the first and second chambers. 7

20 32. A method for testing a plurality of samples,  
comprising (a) simultaneously exposing all samples to a non-  
reactive fluid in a first chamber of a vessel, (b)  
simultaneously exposing all samples in a second chamber of the  
vessel, which is isolated from the first chamber, to a  
25 reactive fluid, and (c) subjecting each sample to analysis.

33. A method according to Claim 32 wherein the analysis  
is optical analysis.

30 34. A method according to Claim 32 wherein the analysis  
is selected from the group consisting of ultrasonic,  
electrostatic, magnetic, radio frequency or x-ray analysis.

35. A method according to Claim 32 wherein each sample is exposed to the reactive fluid in a chamber in which the temperature or the pressure is controlled.

5 36. A method according to Claim 32 wherein each sample is subjected to analysis in a third chamber, and the third chamber is isolated from the first and second chambers.

10 37. A method for testing a group of samples in a sealed vessel, comprising (a) placing one or more members of the group of samples in a position in the vessel to receive separate exposure to a reactive fluid, (b) simultaneously exposing those samples to the fluid, and (c) subjecting in the sealed vessel each member of the group of samples to analysis.

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38. The method of Claim 37 wherein the step of exposing samples to the fluid comprises a step of sliding one component of the sealed vessel relative to another component of the sealed vessel.

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39. A method according to Claim 37 wherein the analysis is optical analysis.

25 40. A method according to Claim 37 wherein the analysis is selected from the group consisting of ultrasonic, electrostatic, magnetic, radio frequency or x-ray analysis.

30 41. A method according to Claim 37 wherein each sample is exposed to the reactive fluid in a chamber in which the temperature or the pressure is controlled.

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43. A method according to Claim 37 wherein each sample is exposed to the reactive fluid in a first chamber, and each

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sample is subjected to analysis in a second chamber, and the first chamber is isolated from the second chamber.

<sup>43</sup>  
~~44~~. An apparatus for testing a group of samples,  
5 comprising (a) a fluid distribution system to simultaneously expose each sample to a reactive fluid, and (b) a holder for the group of samples slidable with respect to the fluid distribution system, and (c) an analyzer.

<sup>44</sup>  
~~45~~. An apparatus according to Claim <sup>43</sup>~~44~~ further  
10 comprising a fluid distribution system to simultaneously expose only the members of a subgroup of the group of samples to a reactive fluid.

<sup>45</sup>  
~~46~~. An apparatus according to Claim <sup>43</sup>~~44~~ wherein the  
15 analyzer performs optical analysis.

<sup>46</sup>  
~~47~~. An apparatus according to Claim <sup>43</sup>~~44~~ wherein the  
20 analyzer performs a method of analysis selected from the group consisting of ultrasonic, electrostatic, magnetic, radio frequency or x-ray analysis.

<sup>47</sup>  
~~48~~. An apparatus according to Claim <sup>43</sup>~~44~~ wherein the  
25 temperature or the pressure is controlled in the reaction chamber in which each sample is reacted with the fluid.

<sup>48</sup>  
~~49~~. An apparatus according to Claim <sup>43</sup>~~44~~ wherein the fluid  
distribution system is isolated from the analyzer.

<sup>49</sup>  
~~50~~. An apparatus for testing a group of samples,  
30 comprising (a) a fluid distribution system to simultaneously expose each sample to a reactive fluid, (b) an analyzer, and

(c) a holder for the group of samples slidable with respect to the analyzer.

5 <sup>49</sup>  
~~50~~ 51. An apparatus according to Claim ~~50~~ further comprising a fluid distribution system to simultaneously expose only the members of a subgroup of the group of samples to a reactive fluid.

10 <sup>49</sup>  
~~51~~ 52. An apparatus according to Claim ~~50~~ wherein the analyzer performs optical analysis.

15 <sup>49</sup>  
~~52~~ 53. An apparatus according to Claim ~~50~~ wherein the analyzer performs a method of analysis selected from the group consisting of ultrasonic, electrostatic, magnetic, radio frequency or x-ray analysis.

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~~53~~ 54. An apparatus according to Claim ~~50~~ further comprising a chamber in which the temperature or the pressure is controlled of each sample is controlled.

<sup>49</sup>  
~~54~~ 55. An apparatus according to Claim ~~50~~ wherein the fluid distribution system is isolated from the analyzer.

25 <sup>55</sup>  
~~55~~ 56. An apparatus for testing a group of samples, comprising (a) a fluid distribution system to simultaneously expose only the members of a subgroup of the group of samples to a reactive fluid, and (b) a holder for the group of samples slidable with respect to the fluid distribution system, and (c) an analyzer.

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~~56~~ 57. An apparatus according to Claim ~~56~~ wherein the analyzer performs optical analysis.

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~~58~~. An apparatus according to Claim ~~58~~<sup>55</sup> wherein the analyzer performs a method of analysis selected from the group consisting of ultrasonic, electrostatic, magnetic, radio frequency or x-ray analysis.
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~~59~~. An apparatus according to Claim ~~58~~<sup>55</sup> wherein the temperature or the pressure is controlled in the chamber in which the member of the subgroup of samples are exposed with the fluid.
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~~60~~. An apparatus according to Claim ~~58~~<sup>55</sup> wherein the fluid distribution system is isolated from the analyzer.
- 60  
~~61~~. An apparatus for testing a group of samples,  
15 comprising (a) a fluid distribution system to simultaneously expose only the members of a subgroup of the group of samples to a reactive fluid, (b) an analyzer, and (c) a holder for the group of samples slidable with respect to the analyzer.
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~~62~~. An apparatus according to Claim ~~61~~<sup>60</sup> wherein the analyzer performs optical analysis.
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~~63~~. An apparatus according to Claim ~~61~~<sup>60</sup> wherein the analyzer performs a method of analysis selected from the group  
25 consisting of ultrasonic, electrostatic, magnetic, radio frequency or x-ray analysis.
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~~64~~. An apparatus according to Claim ~~61~~<sup>60</sup> further comprising a chamber in which the temperature or the pressure  
30 of each member of the subgroup of samples is controlled.
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~~65~~. An apparatus according to Claim ~~61~~<sup>60</sup> wherein the fluid distribution system is isolated from the analyzer.

<sup>65</sup>  
~~66~~. A sealed vessel for testing a plurality of samples,  
comprising (a) a fluid distribution system to simultaneously  
expose the samples to a reactive fluid, and (b) an analyzer in  
the sealed vessel that is isolated from the fluid distribution  
5 system.

<sup>66</sup>  
~~67~~. An apparatus according to Claim <sup>65</sup>~~66~~ wherein the  
analyzer performs optical analysis.

10 <sup>67</sup>  
~~68~~. An apparatus according to Claim <sup>65</sup>~~66~~ wherein the  
analyzer performs a method of analysis selected from the group  
consisting of ultrasonic, electrostatic, magnetic, radio  
frequency or x-ray analysis.

15 <sup>68</sup>  
~~69~~. An apparatus according to Claim <sup>65</sup>~~66~~ wherein the  
temperature or the pressure is controlled in the chamber in  
which each sample is exposed to the fluid.

20 <sup>69</sup>  
~~70~~. An apparatus for testing a plurality of samples,  
comprising (a) a first chamber in which each samples is  
simultaneously exposed to a non-reactive fluid, (b) a second  
chamber, isolated from the first chamber, in which each  
samples is simultaneously exposed to a reactive fluid, and (c)  
an analyzer.

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~~71~~. An apparatus according to Claim <sup>69</sup>~~70~~ wherein the  
analyzer performs optical analysis.

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~~72~~. An apparatus according to Claim <sup>69</sup>~~70~~ wherein the  
analyzer performs a method of analysis selected from the group  
consisting of ultrasonic, electrostatic, magnetic, radio  
frequency or x-ray analysis.

<sup>12</sup>~~72~~. An apparatus according to Claim <sup>69</sup>~~70~~ wherein the fluid distribution system is isolated from the analyzer.

<sup>13</sup>~~73~~. An apparatus for testing a plurality of samples,  
5 comprising (a) a first chamber in which each samples is simultaneously brought to a pre-determined temperature, (b) a second chamber, isolated from the first chamber, in which each samples is simultaneously exposed to a reactive fluid, and (c) an analyzer.

10 <sup>14</sup>~~74~~. An apparatus according to Claim <sup>73</sup>~~74~~ wherein the analyzer performs optical analysis.

<sup>15</sup>~~75~~. An apparatus according to Claim <sup>73</sup>~~74~~ wherein the  
15 analyzer performs a method of analysis selected from the group consisting of ultrasonic, electrostatic, magnetic, radio frequency or x-ray analysis.

<sup>16</sup>~~76~~. An apparatus according to Claim <sup>73</sup>~~74~~ further  
20 comprising a fluid distribution system that is isolated from the analyzer.

<sup>17</sup>~~77~~. An apparatus for testing a plurality of samples,  
comprising (a) a holder for the samples, (b) a cover for the  
25 holder, and (c) an analyzer, wherein the cover is slidable with respect to the holder, and the holder is slidable with respect to the analyzer.

<sup>18</sup>~~78~~. An apparatus according to Claim <sup>77</sup>~~78~~ further  
30 comprising a fluid distribution system to simultaneously expose the samples to a reactive fluid.

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~~80~~. An apparatus according to Claim ~~78~~<sup>77</sup> wherein the analyzer performs optical analysis.

~~80~~  
~~81~~. An apparatus according to Claim ~~78~~<sup>77</sup> wherein the  
5 analyzer performs a method of analysis selected from the group consisting of ultrasonic, electrostatic, magnetic, radio frequency or x-ray analysis.

~~81~~  
~~82~~. An apparatus according to Claim ~~78~~<sup>77</sup> further  
10 comprising a chamber in which the temperature or the pressure is controlled in which each sample is reacted with a fluid.

~~82~~  
~~83~~. An apparatus according to Claim ~~78~~<sup>78</sup> further  
15 comprising a fluid distribution system that is isolated from the analyzer.

~~83~~  
~~84~~. An apparatus for testing a group of samples,  
comprising (a) a fluid distribution system to simultaneously  
expose each sample to a reactive fluid; (b) a reaction  
20 chamber in which each sample is reacted with the fluid, the reaction chamber for each sample being separate and isolated from the reaction chamber for each other sample; and (c) an analyzer.

~~84~~  
~~85~~. An apparatus according to Claim ~~84~~<sup>83</sup> further  
25 comprising a fluid distribution system to simultaneously expose only the members of a subgroup of the group of samples to a reactive fluid.

~~85~~  
~~86~~. An apparatus according to Claim ~~84~~<sup>83</sup> wherein the  
30 analyzer performs optical analysis.

<sup>86</sup>  
~~87~~. An apparatus according to Claim ~~84~~<sup>83</sup> wherein the analyzer performs a method of analysis selected from the group consisting of ultrasonic, electrostatic, magnetic, radio frequency or x-ray analysis.

5 <sup>87</sup>  
~~88~~. An apparatus according to Claim ~~84~~<sup>83</sup> wherein the temperature or the pressure is controlled in the reaction chamber in which each sample is reacted with the fluid.

10 <sup>88</sup>  
~~89~~. An apparatus according to Claim ~~84~~<sup>83</sup> wherein the fluid distribution system is isolated from the analyzer.